

Glutaric acid, 2,6-dimethoxyphenyl tridecyl ester

Inchi:	InChI=1S/C26H42O6/c1-4-5-6-7-8-9-10-11-12-13-14-21-31-24(27)19-16-20-25(28)32-26
InchiKey:	RPTVMYJVVIDDQK-UHFFFAOYSA-N
Formula:	C26H42O6
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]:	450.61

Physical Properties

Property code	Value	Unit	Source
gf	-416.65	kJ/mol	Joback Method
hf	-1120.42	kJ/mol	Joback Method
hfus	64.31	kJ/mol	Joback Method
hvap	100.20	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	6.634		Crippen Method
mcvol	380.060	ml/mol	McGowan Method
pc	888.41	kPa	Joback Method
rinpol	3336.00		NIST Webbook
rinpol	3336.00		NIST Webbook
tb	1028.34	K	Joback Method
tc	1263.49	K	Joback Method
tf	623.02	K	Joback Method
vc	1.468	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1300.73	J/molxK	1028.34	Joback Method
cpg	1357.66	J/molxK	1224.30	Joback Method
cpg	1350.45	J/molxK	1185.10	Joback Method
cpg	1341.17	J/molxK	1145.91	Joback Method
cpg	1329.80	J/molxK	1106.72	Joback Method
cpg	1316.32	J/molxK	1067.53	Joback Method
cpg	1362.80	J/molxK	1263.49	Joback Method
dvisc	0.0000126	Paxs	1028.34	Joback Method

dvisc	0.0000163	Paxs	960.79	Joback Method
dvisc	0.0000217	Paxs	893.23	Joback Method
dvisc	0.0000304	Paxs	825.68	Joback Method
dvisc	0.0000451	Paxs	758.13	Joback Method
dvisc	0.0000725	Paxs	690.57	Joback Method
dvisc	0.0001289	Paxs	623.02	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358715&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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